

Masuda et al. reply: In our original work[1] we reported the observation of an incommensurate ordered state in the frustrated quasi-one-dimensional antiferromagnet LiCu_2O_2 . The Comment by Drechsler *et al.* challenges our conclusions regarding the hierarchy of relevant exchange interactions in the system and the microscopic origin of frustration. In Ref. [1] we postulated a simple model that seemed to explain the available data with only two AF exchange constants $J_1 > J_2 > 0$ (see inset in Fig. 1). Drechsler *et al.* point out that structural arguments and LDA calculations [2] favor a totally different picture [5]: $J_4 > -J_2 > 0$ and $J_1 \sim 0$.

A determination of exchange parameters from bulk data is notoriously ambiguous. To resolve the controversy we have instead recently performed 3-axis inelastic neutron scattering experiments that probe the coupling constants directly [3]. Fig. 1 (symbols) shows the spin wave dispersion measured along the $(0.5, k, 0)$ reciprocal space rod at $T = 1.7$ K. Additional data (not shown) were taken along $(h, 0.827, 0)$ and reveal a sinusoidal dispersion with maxima at integer h values and a bandwidth of 7.5 meV. The measured dispersion curves can be analyzed in the framework of linear spin wave theory (SWT) [4]. It can be shown that in the generalized J_1 - J_2 - J_4 model with inter-chain coupling J_{\perp} there are *exactly two* sets of SWT coupling constants that fit the data: (i) $J_1 = 105$ meV, $J_2 = 34$ meV, $J_4 = -2$ meV and $J_{\perp} = 0.2$ meV and (ii) $J_1 = 6.4$ meV, $J_2 = -11.9$ meV, $J_4 = 7.4$ meV and $J_{\perp} = 1.8$ meV. In the energy range shown in Fig. 1, the spectra calculated from these two models (solid line) are indistinguishable. Solution (i) almost exactly corresponds to our original J_1 - J_2 model. Note, however, that the fitted effective J 's are unrealistically large. While this may merely reflect severe quantum renormalization corrections, the alternative model (ii) appears to be a more likely candidate for LiCu_2O_2 . It incorporates a ferromagnetic J_2 bond, just like the LDA-based model of [2]. However, it involves only *weak* frustration and requires a strong AF J_1 bond, as originally proposed in our work. In addition, the estimated inter-chain coupling constant is smaller than the LDA result by half an order of magnitude. These two discrepancies will have opposite effects on the Curie-Weiss temperature, which could in turn explain why the LDA-based model still yields reasonable estimates of this quantity.

Trying to reconcile the result by Drechsler *et al.* with the measured dispersion of spin waves, we note that *just the data taken along* $(0.5, k, 0)$ can be also perfectly reproduced by $J_1 = 0$, $J_2 = -10$ meV, $J_4 = 7$ meV and $J_{\perp} = 8$ meV. This set of parameters is at least qualitatively consistent with their model. However, with these numbers SWT gives an *a*-axis bandwidth of 13 meV, almost twice as large as observed. One possibility is that Drechsler's model is actually correct, but SWT breaks down *qualitatively*, and can not give correct excitation energies in the entire Brillouin zone *even using some ef*

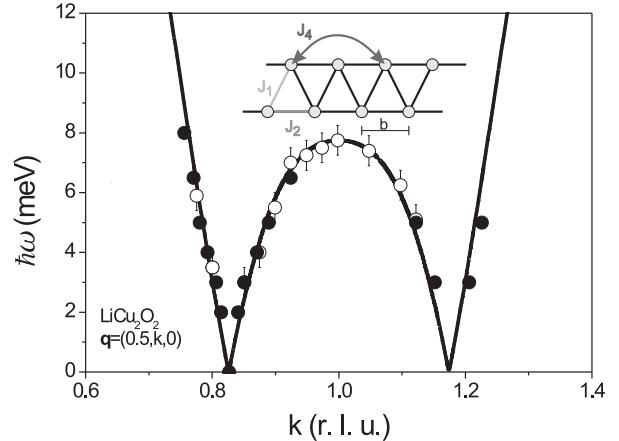


FIG. 1: Spin wave dispersion in LiCu_2O_2 measured using constant- E (solid symbols) or constant- Q scans (open symbols). Lines are as described in the text.

fective set of renormalized coupling constants. This intriguing possibility deserves a closer theoretical investigation, but seems unlikely. Indeed, in LiCu_2O_2 the suppression of T_c is not too pronounced, and a renormalized quasiclassical picture should work rather well.

In summary, the frustration mechanism in LiCu_2O_2 is more complex than we originally thought, and involves a *ferromagnetic* J_2 bond. However, our present understanding of the inelastic neutron scattering results suggests a strong “rung” interaction J_1 and weak inter-chain coupling, in contradiction with the model of Drechsler *et al.* This work was partially supported by the Civilian Research and Development Foundation project RU-P1-2599-04. Work at ORNL was supported by the U. S. Department of Energy under Contract No. DE-AC05-00OR22725.

T. Masuda[†], A. Zheludev[†], A. Bush[‡], M. Markina[‡], and A. Vasiliev[‡]

[†] Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6393, USA.

[‡] Moscow Institute of Radiotechnics, Electronics and Automation, Moscow 117464, Russia.

[§] Low Temperature Physics Department, Moscow State University, Moscow 119992, Russia.

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- [2] A. A. Gippius *et al.*, Phys. Rev. B **70**, Rapid Comm., in press (2004), cond-mat/0312576.
- [3] T. Masuda, A. Zheludev, B. Roessli, A. Bush, M. Markina and A. Vasiliev, in preparation.
- [4] T. Nagamiya, Solid State Physics, Academic Press, New York, 1967, Vol. 20, p. 305.
- [5] Drechsler *et al.* use a different notation, related to ours through $J_1 \rightarrow J_{\text{DC}}$, $J_2 \rightarrow J_1$ and $J_4 \rightarrow J_2$.